Searching for a higher superconducting transition temperature in strained MgB_2

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We present a detailed first-principles density-functional analysis of the effects of lattice strain on the superconducting transition temperature, T_c, of MgB_2, deriving a general rule that governs the enhancement (or suppression) of T_c in strained MgB_2 in terms of electronic and phonon contributions. Based on the calculated structural, electronic, vibrational, and superconducting properties of a strained MgB_2 superconductor, we show how a higher T_c might be achieved. Several candidate substrates are suggested for growing MgB_2 thin films to gain a higher T_c.

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Tailoring the T_c in MgB_2 requires a full atomic level understanding of the underlying mechanism of chemical and lattice effects. Immediately after the discovery of superconductivity in MgB_2,[1] extensive research on chemical substitution was undertaken to understand and hence to improve its properties.[2–5] In contrast, very few studies focused on lattice effects despite the fact that improving material properties by controlling lattice strain is a basic and practical approach in materials research. For example, various methods, such as applying pressures[6,7] including mechanical loads, or selecting different substrates with different lattice constants for film growth, are commonly employed to investigate the effects of lattice strain on material functionality. Lattice effects are believed to play an important role in the superconductivity of MgB_2. Although isotropic compression was applied to the crystal lattice of MgB_2 to investigate its properties,[6,7] no research has systematically addressed the effects of strain on superconductivity. In fact, various strains exist in epitaxially grown MgB_2 films due to the use of different substrates. Very encouragingly, Pogrebnyakov *et al.*, reported that the T_c of MgB_2 can be increased by as much as about 5% using SiC as the substrate.[8] Seemingly, a thorough exploration of the effects of both compressive and tensile strains on the superconducting properties of MgB_2 would be extremely useful for guiding the way toward a higher T_c. In this paper, we discuss the effects of lattice strain on the electronic (density of states and deformation potential), vibrational (E_{2g} phonon), and superconducting (T_c) properties in MgB_2 using density functional theory (DFT).[9]

We first describe the variation of T_c as a function of strain in a way generalized for low-temperature superconductors and then specify them for strained MgB_2. The original McMillan formula[10] for T_c of superconductor is given as

$$T_c = \frac{\Theta}{1.45} \exp\left[- \frac{1.04(1+\lambda)}{\lambda(1-0.62\mu^*) - \mu^*} \right], \qquad (1)$$

where Θ is Debye temperature, μ^* is the Coulomb pseudopotential, and λ is electron-phonon coupling strength. The Allen-Dynes[11,12] modified McMillan formula can be expressed as

$$T_c = \frac{\omega_{\log}}{1.2} \exp\left[- \frac{1.04(1+\lambda)}{\lambda(1-0.62\mu^*) - \mu^*} \right]. \qquad (2)$$

The Debye temperature Θ in Eq. (1) and $\omega_{\log}$ in Eq. (2) are related to phonon frequencies. According to Morel and Anderson,[13] μ^* can be expressed as

$$\mu^* = \frac{\mu}{1 + \mu \ln(E_F/\omega)}, \qquad (3)$$

where $\mu = 0.5 \ln[(1+g^2)/g^2]$ and $g^2 = \pi e^2 N_F / k_F^2$. Here, $k_F = (3\pi^2 Z/V)^{1/3}$, where Z is the valency and V is the volume.[14] The electron-phonon coupling strength λ can be expressed as

$$\lambda = \frac{N_F \langle I^2 \rangle}{M\langle \omega^2 \rangle} = \frac{\eta}{M\langle \omega^2 \rangle}, \qquad (4)$$

where N_F is density of states (DOS) at Fermi energy level, $\langle I^2 \rangle$ is the mean-square electron-ion matrix element, M is the ionic mass, $\langle \omega^2 \rangle$ is the mean-square phonon frequency, and η is McMillan-Hopfield parameter that includes the electronic components of electron-phonon coupling. In a strained superconductor, the relative change of T_c as a function of strains can be expressed as

$$\frac{\Delta T_c}{T_{c0}} = \frac{\Delta \omega_{\log}}{\omega_{\log}} - \alpha \frac{\Delta \mu^*}{\mu_0^*} + \beta \frac{\Delta \lambda}{\lambda_0}. \qquad (5)$$

All variables with subscript 0 are for a strain-free superconductor, and the strain-free parameters are

$$\alpha = \frac{1.04(1+\lambda_0)(1+0.62\lambda_0)\mu_0^*}{[\lambda_0(1-0.62\mu_0^*) - \mu_0^*]^2}$$

and

$$\beta = \frac{1.04\lambda_0(1+0.38\mu_0^*)}{[\lambda_0(1-0.62\mu_0^*) - \mu_0^*]^2}.$$

To achieve higher T_c in terms of modulating the strain, the following condition should be fulfilled:

$$\frac{\Delta \omega_{\log}}{\omega_{\log}} - \alpha \frac{\Delta \mu^*}{\mu_0^*} + \beta \frac{\Delta \lambda}{\lambda_0} > 0. \quad (6)$$

Equations (5) and (6) are general ones for low-temperature superconductors where the McMillan-Allen-Dynes formula can be applied. The above terms can be obtained from DFT calculations to give T_c as a function of strains.

Next, we specify how to achieve a higher T_c in strained MgB_2. It is well known that MgB_2 is a two-band superconductor.[15–18] The T_c of MgB_2 is derived from both the 2D σ and 3D π bands components, but is dominated by the boron 2D σ band.[15] The boron 2D σ band and the E_{2g} phonon frequency (boron-boron stretching mode), as well as the deformation potential associated with this mode, are mainly responsible for the interesting superconducting properties of MgB_2. In a small range ($\pm 6\%$) of strains, the variation of T_c is mainly determined by modulations of the σ band. Therefore, in this paper, we will focus on the variations in the electronic and phonon parts of the σ band and their effects on T_c in strained MgB_2.

In this case, $\omega_{\log}$ is approximately proportional to the E_{2g} phonon frequency $\omega_{E_{2g}}$, and electron-phonon coupling can be expressed[19] as $\lambda \propto N_F(\sigma)|D|^2/M_B\omega_{E_{2g}}^2$, where M_B is atomic mass of boron, $|D|$ is the deformation potential associated with the boron-boron bond stretching mode, and $N_F(\sigma)$ is the density of states of the boron σ band at the Fermi level.[19] In strained MgB_2, a small deviation in Δa and Δc of the lattice constants a_0 and c_0 results in the variation of λ, $\omega_{E_{2g}}$, μ^*, and T_c. The changes of T_c can be expressed as

$$\frac{\Delta T_c}{T_{c0}} = \frac{\Delta \omega_{E_{2g}}}{\omega_{E_{2g0}}} - \alpha \frac{\Delta \mu^*}{\mu_0^*} + \beta \frac{\Delta \lambda}{\lambda_0}, \quad (7)$$

where

$$\frac{\Delta \lambda}{\lambda_0} = \frac{\Delta N_F(\sigma)}{N_{F0}(\sigma)} + \frac{2\Delta|D|}{|D|_0} - 2\frac{\Delta \omega_{E_{2g}}}{\omega_{E_{2g0}}}. \quad (8)$$

The first-principles DFT calculations were made using the full potential augmented plane wave (FPAPW) method implemented in the *WIEN2k* package,[20] and the plane-wave pseudopotential method in the *ABINIT* package,[21] respectively. For both methods, we employed the local density approximation (LDA) suggested by Perdew and Wang,[22] and the generalized gradient approximant (GGA) proposed by Perdew, Burke, and Ernzerhof (PBE96)[23] to obtain the exchange-correlation potential. The results from the LDA and GGA agree well with each other with difference within 2%. For full potential calculations (*WIEN2k*), a muffin-tin radius (R_{MT}) of 1.7 bohr was chosen for Mg, and 1.5 bohr for B, and $R_{MT}K_{max}$ was taken to be 8.0. The calculations used the angular momentum expansion up to $l_{max}=10$ for the potential and charge density representations. At convergence, the integrated difference between input and output charge densities (atomic unit) was less than 10^{-5}. We also employed 3000 k points in the Brillouin zone in the calculations. (The convergence of total energy and properties of MgB_2 was tested in terms of the number of k points.) In pseudopotential calculations (*ABINIT*), we employed a very large energy cutoff (40 Hartree) and $10\times10\times10$ Monkhorst-Pack[24] k points, and a very small tolerance on the potential $V(r)$ residual (10^{-18}) for self-consistent field (SCF) stopping; this ensured good convergence of the results in ground-state and linear-response calculations. Well-tested Troullier-Martins pseudopotentials[25] were adopted.

With the chosen typical value $\mu_0^*=0.15$, and $\lambda_0=0.94$, as well as our calculated phonon frequency $(\omega_{E_{2g}})_0 = 579.9\ \mathrm{cm}^{-1}$, we obtain $T_{c0}=39.4$ K for bulk MgB_2 with the lattice constant $a=3.083$ Å, $c=3.521$ Å, agreeing with experimental data.[1] We note that the changes in superconducting properties (e.g., T_c) as a function of strains are mainly determined by the *relative* changes of ω, λ, and μ^* (which are, in turn, determined by the relative changes of ω, N_F, and D), while the actual values of μ_0^* and λ_0 are less sensitive to the strain-induced variation of T_c in MgB_2. This can be demonstrated by Eqs. (7) and (8), in which we express the variation of T_c relative to T_{c0} based on the relative changes of ω and λ. Other coefficients that are associated with λ and independent of ω, N_F, and D are cancelled out in the ratio of $\Delta\lambda/\lambda_0$. We show numerical results later in this work, demonstrating that the trends in the superconducting properties of MgB_2 as a function of strains are not affected significantly by the choice of μ_0^* and λ_0.

The change of μ^* in strained MgB_2 is rather small and is only about ten times less than the relative changes of λ, which is consistent with Chen *et al.*'s findings[26] for MgB_2 under hydrostatic pressure. Using our calculated value of $\alpha \sim 0.97$, the contribution of the $-\alpha\Delta\mu^*/\mu_0^*$ term modifies $\Delta T_c/T_{c0}$ by about 1%–2% in the range of strains described in this work. Hereafter, the term of $\Delta\mu^*/\mu_0^*$ will not be included explicitly.

We note that the T_c of MgB_2 is controlled collectively by three components: phonon frequency $(\Delta\omega/\omega_0)$, density of states $[\Delta N_F(\sigma)/N_{F0}(\sigma)]$, and the deformation potential $(2\Delta|D|/|D|_0)$. By sorting out the individual contributions and defining the electron contribution $\delta_e = \Delta N_F(\sigma)/N_{F0}(\sigma) + 2\Delta|D|/|D|_0$, and the phonon contribution $\delta_p = \Delta\omega/\omega_0$, we derive a simple expression,

$$\delta_{T_c} = \frac{\Delta T_c}{T_{c0}} = \beta\delta_e + (1-2\beta)\delta_p, \quad (9)$$

where the subscripts e and p indicate the contribution from the electron and phonon component, respectively. For the strain-free bulk, we obtain the parameter $\beta=2.09$; then, $\delta_{T_c}=2.09\delta_e-3.18\delta_p$. This clearly demonstrates that the contributions from the electron and phonon parts can be considered as two separate competing entities, i.e., δ_{T_c} increases with an increase in δ_e but with a decrease in δ_p, and vice versa.

Thus, to improve the T_c in strained MgB_2, the following condition should be fulfilled:

$$\delta_{T_c} > 0 \quad \text{or} \quad \delta_e > \frac{(2\beta-1)}{\beta}\delta_p \approx 1.52\delta_p. \quad (10)$$

This simple rule indicates the general direction to take for enhancing the T_c of MgB_2: no matter whether the E_{2g} pho-

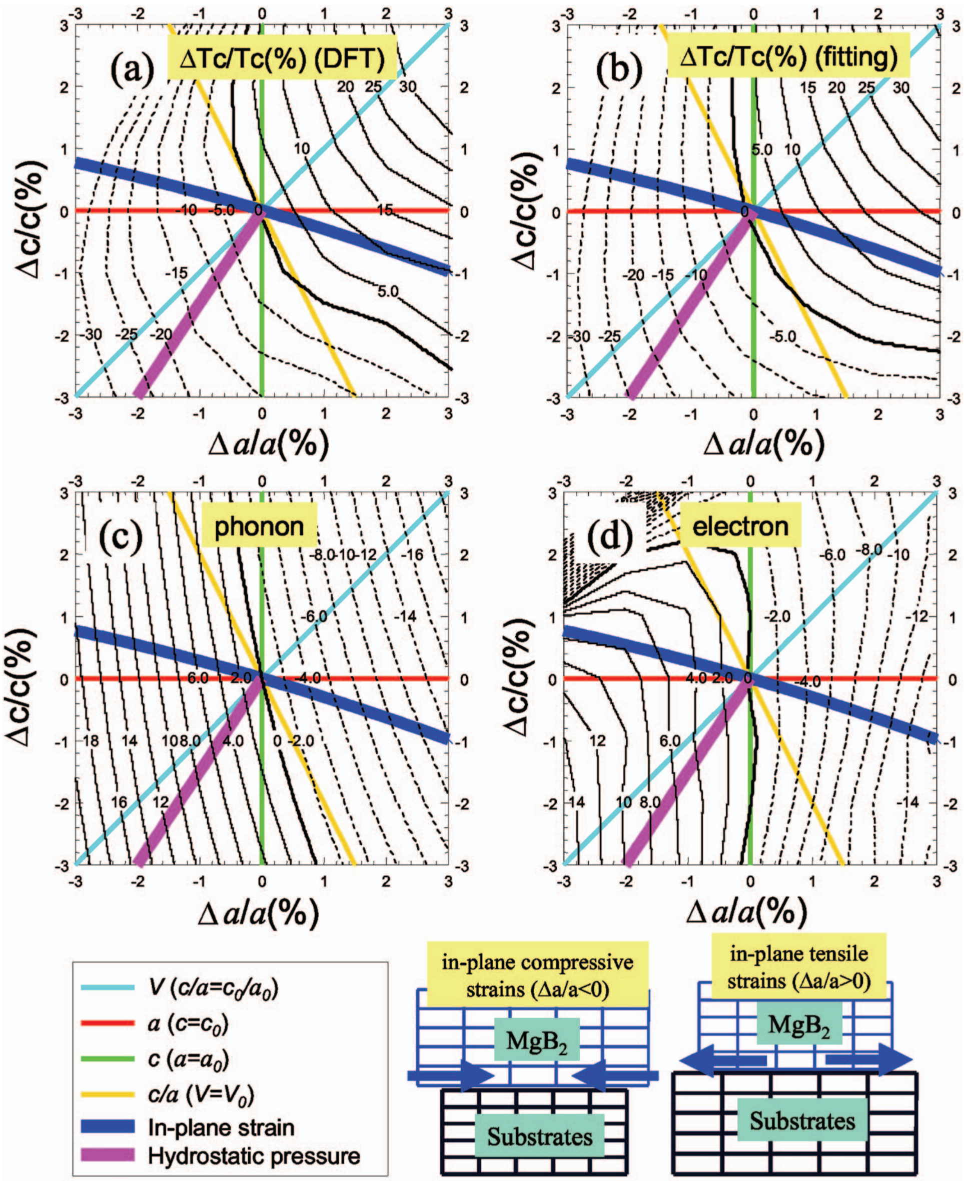

FIG. 1. (Color) 2-D contour plot of critical temperature and its associated electron and phonon contributions in MgB_2 as a function of variation of lattice constants. (a) Critical temperature ($\Delta T_c/T_c$) obtained from DFT calculations. (b) Critical temperature obtained by fitting DFT results using Eq. (11). (c,d) Phonon and electron contributions to $\Delta T_c/T_c$. The colored lines indicate different variations as a function of $\Delta a/a$ and $\Delta c/c$ in MgB_2 (cyan: volume variation V with fixed c/a; red: variation of lattice constant a with fixed c; green: variation of lattice constant c with fixed a; yellow: variation of c/a with fixed volume; bold blue line: lattice variation for in-plane strain; bold red line: lattice variation for hydrostatic pressure up to 12 GPa). The solid and dashed counter-lines represent positive and negative $\Delta Tc/Tc$, respectively. Schematics of MgB_2 films with in-plane compressive and tensile strains grown on substrates are shown at the bottom right.

non is softened or strengthened, if the electron contribution, δ_e, is greater than $1.52\delta_p$, T_c can be raised.

So far, we have clarified the underlying mechanism of variation for T_c in terms of the contributions of electrons and phonons. However, in searching for a higher critical temperature in strained MgB_2, it is worth looking at their detailed behavior as a function of the strains. In Fig. 1, we plot δ_{Tc} vs. $\Delta a/a$ $(-3\%-3\%)$, and $\Delta c/c$ $(-3-3\%)$, in MgB_2. We found that by increasing $\Delta a/a$ and $\Delta c/c$ the T_c can be raised (solid line counters in Fig. 1), as is even more evident from the variation of T_c vs. $\Delta a/a$ (or $\Delta c/c$) with a fixed $\Delta c/c$ (or $\Delta a/a$). The most significant way of increasing T_c is by increasing the volume, V, of MgB_2 with a fixed c/a. The origin of this enhancement is the decrease in both the phonon and electron contributions, namely, $\delta_p<0$ and $\delta_e<0$ with $\delta_e>1.52\delta_p$, as shown in Figs. 1(c) and 1(d). Using the results of our DFT calculations, a simple coupling quadratic fitting to DFT data was obtained using

$$\delta_{\mathrm{Tc}} = a_1x + a_2x^2 + b_1y + b_2y^2 + c_1xy, \tag{11}$$

where $x=\Delta a/a$, and $y=\Delta c/c$. The quality of the fit is excellent with the following fitting parameters: $a_1=9.836\,028$, $a_2=-0.865\,501$, $b_1=2.782\,717$, $b_2=-0.642\,597$, and $c_1=1.786\,229$ [Figs. 1(a) and 1(b)]. The importance of this fitting formula is that once the strain condition ($\Delta a/a$ and $\Delta c/c$) in MgB_2 is known, δ_{Tc} can be predicted directly, and, thus, by using $T_c=T_{c0}\cdot(1+\delta_{Tc})$, where $T_{c0}=39.4$ K is the value of unstrained MgB_2, T_c can be obtained without needing expensive DFT calculations.

We now compare the calculated δ_{Tc} both from DFT calculations and the fitting formula Eq. (11) with that from experimental data for two typical cases in MgB_2: (*i*) bulk material with uniaxial pressure (Figs. 1 and 2) and (*ii*) thin films grown on different substrates (Figs. 1 and 3). With hydrostatic pressure, both the lattice constants a and c are compressed (bold red line in Fig. 1), and δ_{Tc} falls as the lattice

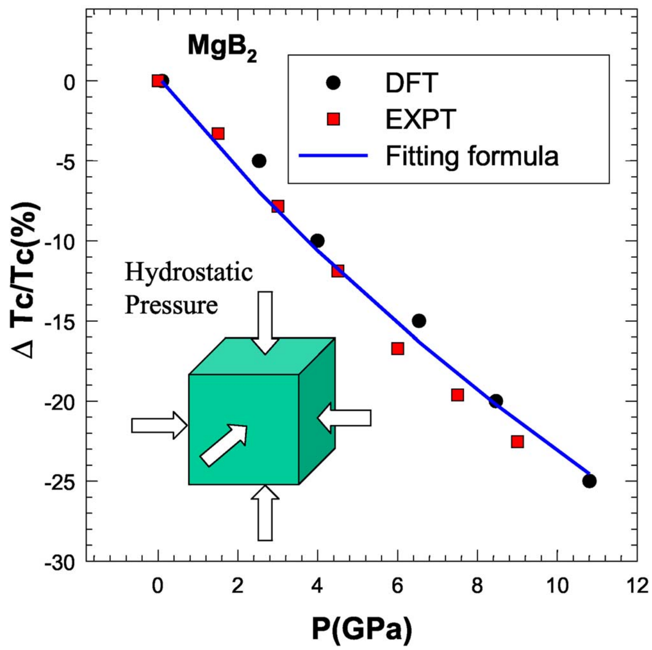

FIG. 2. (Color online) Comparison of critical temperature between experiments and the DFT calculation of MgB_2 as a function of hydrostatic pressure. The solid line is from the fitting formula [Eq. (11)]. The experimental data is taken from Ref. 7.

constants decrease. Figure 2 compares the experimentally measured δ_{Tc} as a function of applied pressure with the results of DFT calculations and with Eq. (11); there is excellent agreement between the three. We conclude that applying hydrostatic pressure always leads to a drop in T_c.

A higher T_c can be attained in MgB_2 thin film under biaxial strain in the a-b basal plane (in-plane), as depicted in Fig. 1 (bold blue line) and Fig. 3(a). Furthermore, the optimized variation in lattice constant, $\Delta c/c$, determined from minimizing total energy, declines slightly with an increase in $\Delta a/a$ with a negative slope close to $-1/3$. The calculated δ_{Tc} in strained MgB_2 from DFT agrees well with the experimental values[8] using SiC as a substrate [Fig. 3(a)]. The δ_{Tc} predicted from the fitting formula [Eq. (11)] is consistent with the measured δ_{Tc} with an error of about -2% (the same order as the experimental error bar). Our results are striking because not only do they agree with the experiments, but they also reveal the possibility of further improving T_c by using large tensile strains [1% to 3%, Fig. 3(a)]. The enhancement of T_c originates from the decrease in the phonon (δ_p) and electron (δ_e) contributions due to the increase in biaxial strains [see Fig. 3(c)] that satisfy the condition of Eq. (10) in the 3% range of strains. Our finding that decreasing the E_{2g} phonon frequency [Fig. 3(c)] will generate a high T_c in MgB_2 agrees well with the experimental observations and

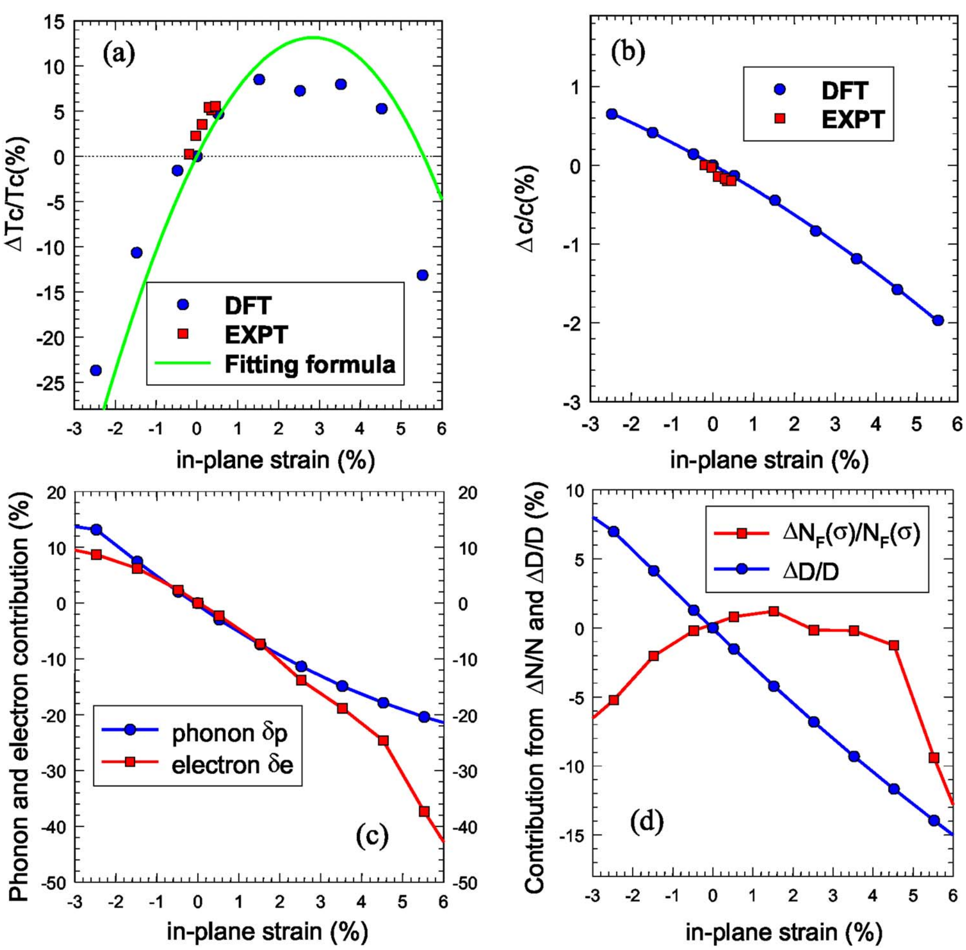

FIG. 3. (Color online) The critical temperature and other variables in MgB_2 as a function of in-plane biaxial strains. (a) Critical temperature $\Delta T_c/T_c$, (b) lattice variation $\Delta c/c$, (c) electron [$\delta_e = \Delta N_F(\sigma)/N_F(\sigma) + 2\Delta D/D$, red squares] and phonon ($\delta_p = \Delta\omega/\omega$, blue dots) contribution, and (d) boron σ band density of state $\Delta N_F(\sigma)/N_F(\sigma)$ (red squares) and deformation potential $\Delta D/D$ (blue dots).

theoretical predictions:[8] i.e., the softened Raman phonon peak in strained MgB_2 gives a higher T_c.

Our calculations further demonstrate that the δ_{Tc} in MgB_2 increases with rising biaxial strains until reaching its maximum of about 10%, at ~3% tensile strains; thereafter, it decreases with any further rise in tensile strains and then falls to a negative value at very high strains (~6% or more). The reason this occurs is that Eq. (10) is not fulfilled: thus, although both δ_p and δ_e decline, δ_e decreases at a rate faster than $1.52\delta_p$. The fall in T_c at high tensile strains reflects the sharp decrease of density of states of the B σ band, $N_F(\sigma)$ [Fig. 3(d)].

Taking into account both δ_{Tc} and strained energy in MgB_2, we found there is still plenty of room for raising T_c to higher value: if biaxial strains of about 1%–3% can be achieved, the T_c can be enhanced by about 7%–12% (corresponding to $T_c = 42-44$ K). So, the question is how to increase biaxial strains. This problem can be resolved by selecting appropriate substrates for growing MgB_2 thin films that have a slightly larger lattice constant than that of bulk (or unstrained) MgB_2, or applying biaxial tensile stress with a mechanical load in a single crystal. There are several possible substrates: hexagonal SiC, $Si_{1+x}C_{1-x}$ alloys with a small tunable composition x, to vary lattice constant, AlN, GaN and their alloys $Al_xGa_{1-x}N$, as well as MgB_2 doped with Ca (or $Mg_{1-x}Ca_xB_2$ alloys). All these materials have a slightly larger biaxial lattice constant than does bulk MgB_2 at low temperatures, and, as substrates for MgB_2, they will generate tensile strains in the films. In particular, if high-quality MgB_2 films can be grown on alloys of $Si_{1+x}C_{1-x}$, $Al_xGa_{1-x}N$, or $Mg_{1-x}Ca_xB_2$, then, by controlling the composition x of the alloy substrates, the tensile strains, and, thus, T_c can be tuned. For materials that have lattice constants comparable with (or even smaller than) those of MgB_2 at room temperature, for example, 6H–SiC ($a = 3.0806$ Å at 300 K),[27] it still is possible to induce tensile strains by cooling the sample to below the T_c of MgB_2 because the thermal coefficient of MgB_2 (5.4×10^{-6} K^{-1})[28] is about twice as large as that of SiC (2.77×10^{-6} K^{-1}),[27] resulting in a small tensile strain for MgB_2 at low temperatures on a SiC substrate. For AlN with its wurtzite structure, its lattice constant ($a = 3.111$ Å)[27] is slightly larger than that of MgB_2, but its thermal expansion coefficient (4.2×10^{-6} K^{-1})[29] is less. Therefore, by growing MgB_2 on an AlN substrate, the tensile strains in the films (~1%) will be larger than those (~0.5%) of films grown on a SiC substrate, and accordingly, the T_c of MgB_2 will be enhanced by about 7%–8%.

Finally, we discuss the validation of our approach. Although we used some approximations (for example, the McMillan-Allen-Dynes formula for T_c, the variation of μ^* in strained MgB_2 is neglected) in calculating T_c in the strain-induced modulation of MgB_2, the excellent agreement between the calculated and experimental T_c for MgB_2 in two typical cases (applied hydrostatic pressure and tensile strain) justifies the validity of this approach and suggests that the superconducting properties of MgB_2 as a function of strains are mainly dominated by the strain-induced modulation of the σ band (e.g., density of states, deformation potentials, E_{2g} phonon frequency). In fact, the McMillan-Allen-Dynes formula has been used for calculating T_c MgB_2 in many cases, for example, for bulk MgB_2,[19,30,31] MgB_2 under pressure,[26,32] MgB_2 doped with carbon,[33] or aluminum[34] and strained MgB_2.[8] Another concern centers on the effects of the selected values of μ_0^* and λ_0 on the strain-induced modulation of T_c. It was found that the trends of superconducting properties of MgB_2 as a function of strains are not affected significantly by the choice of μ_0^* and λ_0. We proved this point by using a wide range of values of μ_0^* and λ_0, with μ_0^* being 0.1–0.2, and λ_0 being 0.6–1.0, for strain-free MgB_2 to reproduce $T_c = 39.4$ K. As clearly demonstrated in Fig. 4, the $\Delta T_c / T_{c0}$ of strained MgB_2 is insensitive to the values of μ_0^* and λ_0. It is worth mentioning that our method describes the relative changes of T_c in terms of relative changes of related physical quantities and, therefore, it will have more precision than the straight calculation of the absolute value of T_c by using the McMillan-Allen-Dynes formula on MgB_2, an anisotropic and anharmonic two-band material.

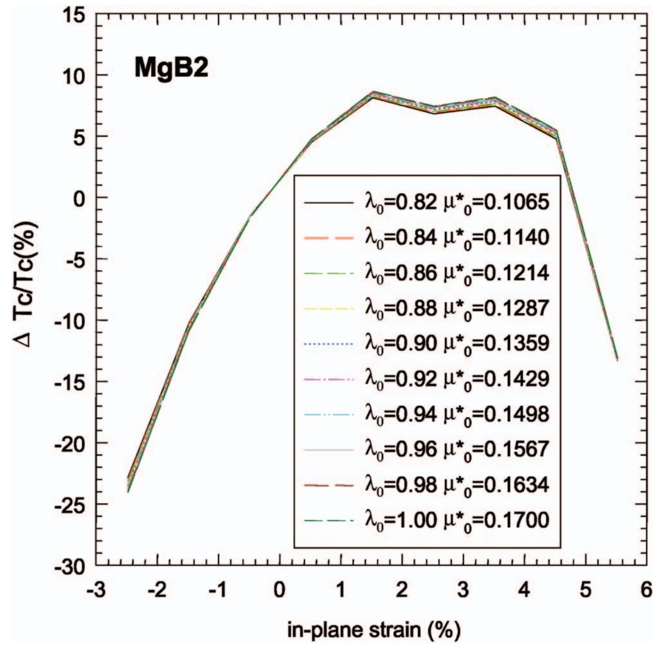

FIG. 4. (Color) $\Delta T_c / T_c$ as a function of in-plane strain for a wide range of μ_0^* and λ_0. (Color represents different values of μ_0^* and λ_0.)

In summary, we used first-principles DFT calculations to determine the electronic, vibrational, and superconducting properties of MgB_2 under various conditions of strain. We derived a general rule governing the enhancement (or suppression) of T_c in strained MgB_2 in terms of electron and phonon contributions. Based on this rule, we found that the direction of increasing T_c should lie in efforts to increase tensile strains (from 0% up to 4%). The maximum T_c in strained MgB_2 may be achieved at tensile strains of 2%–3%. Several candidate substrates for growing MgB_2 thin films were suggested. We emphasize that our rule is not limited to MgB_2, but is applicable to other conventional BCS superconductors (with different values of β), especially those having similar lattice structures to MgB_2. Our approach to strain engineering, with the target of enhancing T_c as demonstrated in this work, can be applied to various strain-engineering problems in other functional materials. In fact, we have demonstrated, by first-principles calculations, that half-metallic ferromagnetism (an important property for spintronics) can be enhanced in strained zinc-blende structures of MnSb and MnBi.[35]

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